

C₂ IN PECULIAR DQ WHITE DWARFSPATRICK B. HALL,¹ AARON J. MAXWELL¹*Submitted to ApJ Nov. 25, 2007; Accepted Jan. 29, 2008*

ABSTRACT

White dwarfs (WDs) with carbon absorption features in their optical spectra are known as DQ WDs. The subclass of peculiar DQ WDs are cool objects ($T_{\text{eff}} \lesssim 6000$ K) which show molecular absorption bands that have centroid wavelengths $\sim 100\text{--}300$ Å shortward of the bandheads of the C₂ Swan bands. These “peculiar DQ bands” have been attributed to a hydrocarbon such as C₂H. We point out that C₂H does not show strong absorption bands with wavelengths matching those of the peculiar DQ bands and neither does any other simple molecule or ion likely to be present in a cool WD atmosphere. C₂ seems to be the only reasonable candidate for producing the peculiar DQ bands. Many characteristics of those bands can be understood if they are pressure-shifted Swan bands. While current models of WD atmospheres suggest that, in general, peculiar DQ WDs do not have higher photospheric pressures than normal DQ WDs do, that finding requires confirmation by improved models of WD atmospheres and of the behavior of C₂ at high pressures and temperatures. If it is eventually shown that the peculiar DQ bands cannot be explained as pressure-shifted Swan bands, the only explanation remaining would seem to be that they arise from highly rotationally excited C₂ ($J_{\text{peak}} \gtrsim 45$). In either case, the absorption band profiles can in principle be used to constrain the pressure and the rotational temperature of C₂ in the line-forming regions of normal and peculiar DQ WD atmospheres, which will be useful for comparison with models. Finally, we note that progress in understanding magnetic DQ WDs may require models which simultaneously consider magnetic fields, high pressures and rotational excitation of C₂.

Subject headings: white dwarfs, stars: atmospheres, molecular processes

1. INTRODUCTION

Carbon white dwarfs (DQ WDs) with $T_{\text{eff}} \lesssim 11000$ K can show absorption from the Swan bands of C₂. Peculiar carbon white dwarfs (DQ PEC or DQp WDs) are relatively cool WDs ($T_{\text{eff}} \lesssim 6000$ K) which exhibit bands reminiscent of the Swan bands, but with more rounded profiles and with centroid wavelengths located $\sim 100\text{--}300$ Å (700 ± 100 cm⁻¹) shortward of the bandheads of the Swan bands (Table 1; see also Figure 3 of Schmidt, Bergeron, & Fegley 1995 and Figure 30 of Bergeron, Ruiz, & Leggett 1997). The origin of these “peculiar DQ bands” or DQp bands has been a matter of some debate. Liebert & Dahn (1983) first suggested they were pressure-shifted Swan bands, but Bergeron et al. (1994) cast doubt on that interpretation (see § 3.2). Strong magnetic fields can and do distort the Swan bands in some carbon WDs, but the DQp WDs are not all strongly magnetic (Schmidt et al. 1995, 1999), so another explanation is required for their bands. One well-received explanation was put forward by Schmidt et al. (1995), who attributed the DQp bands to a hydrocarbon such as C₂H rather than to C₂. As a result, DQp WDs have also been referred to as C₂H WDs. However, until the origin of the bands in such objects is conclusively settled, we prefer to use the nomenclature of DQp WDs and DQp bands.

In this contribution we report an unsuccessful literature search for known transitions from C₂H and other simple molecules that correspond to the DQp bands (§ 2). We then revisit the issue of how C₂ might produce the DQp bands (§ 3). We summarize our conclusions in § 4.

2. THE PECULIAR DQ BANDS: EXPLANATIONS BESIDES C₂2.1. *Ruling Out C₂H*

Motivated by the abundance analysis of LHS 1126 by Bergeron et al. (1994), Schmidt et al. (1995) suggested that DQp WDs have relatively large amounts of hydrogen ($\gtrsim 10\%$ of the helium abundance, compared to $\sim 0.1\%$ in normal DQ WDs). Under such conditions, neither C₂ nor CH will be the most abundant carbon-hydrogen molecule. Instead, Schmidt et al. (1995) suggested that the DQp bands arise in C₂H, which was generally the most abundant such molecule in their models.

Schmidt et al. (1995) were not aware of theoretical or observational work on the optical spectrum of C₂H, but such work does exist. In fact, Perić, Peyerimhoff, & Buenker (1992) cite 39 experimental and 13 theoretical investigations of C₂H. In particular, Graham, Dismuke, & Weltner (1974) show that C₂H does not produce bands similar to the C₂ Swan bands. The C₂H molecule is electronically more like CN and has bands only at $\lambda < 3400$ Å, $8670 \text{ Å} < \lambda < 8750$ Å and $\lambda > 9430$ Å. In no other study cited by Perić et al. (1992) has experimental or theoretical evidence been reported for bands of C₂H in the range 4000–6000 Å.

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TABLE 1
SWAN AND DQP BAND SYSTEM PARAMETERS

Swan Band Δv	Swan Band Bandhead, Å	DQP Band Centroid, Å	ΔE , cm^{-1}
+4	3828
+3	4083
+2	4382	4280	+549
+1	4737	4575	+748
0	5165	5000	+639
-1	5636	5400	+775
-2	6191	5900	+797
-3	6857
-4	7670

This fact was mentioned by Jørgensen et al. (2000), who concluded that “the likelihood of C_2H being responsible for [the DQP bands] ... is very small.” However, in our opinion the wealth of previous research on C_2H means that C_2H has no chance of being responsible for the peculiar DQ bands. For example, even if previously unknown and unsuspected transitions of C_2H matching the DQP bands exist, if C_2H is prominent in DQP WDs we should expect such WDs to exhibit 8710 Å band absorption from C_2H molecules in the ground state. Such absorption has not been reported in the literature, nor is it seen in the spectra of DQP WDs catalogued by Harris et al. (2003), Dufour, Bergeron, & Fontaine (2005), Koester & Knist (2006) or Eisenstein et al. (2006).

2.2. Ruling Out Other Molecules

Schmidt et al. (1995) explored molecule formation in atmospheres with an H/He abundance ratio of 0.1 and C/He abundance ratios down to 10^{-5} . Depending on the temperature and pressure, they found that a number of simple hydrocarbon molecules could be most abundant, such as CH, C_2H , C_2H_2 or CH_2 . We have searched the literature extensively and have ruled out these and other molecules as being responsible for the DQP bands, either because the molecules have no permitted optical transitions or because they have ones whose wavelengths do not match those of the DQP bands. The following molecules and ions are ruled out by the following references: C_2^+ (Maier & Rösslein 1988), CH (Herzberg & Johns 1969), CH_2 (Herzberg & Shoosmith 1959), CH_3 (Herzberg & Johns 1966), CH_4 (Giver 1978), C_2H_2 (Lundberg et al. 1993), C_2H_3 (Pibel et al. 1999; Pushkarsky et al. 2001; Shahu et al. 2002), C_2H_4 (Adel & Slipper 1934), C_2H_6 (Dick & Fink 1977), C_3 (Fix 1976), C_3H (Ding et al. 2001), C_5 (Hanrath & Peyerimhoff 2001), C_5H , C_7H and C_9H (Ding et al. 2002). Lastly, since it is possible that oxygen and even nitrogen as well as carbon could be present in the atmospheres of cool WDs (Hansen & Liebert 2003; Jørgensen et al. 2000), we have ruled out the following molecules containing O or N as potential explanations for the DQP bands: HCO (Dixon 1969), C_2O (Choi et al. 1998), CO (Herzberg 1950), O_2 (Herzberg 1950), OH (Dieke & Crosswhite 1962), H_2O (Herzberg 1966), CN (Herzberg 1950) and HCN (Schwenzer et al. 1974).

A few molecules deserve special note.

We rule out absorption from metastable He_2 , as suggested by Aslan & Bues (1999). He_2 does produce three broad optical absorption bands, but their wavelengths do not match those of the peculiar DQ bands (Brooks & Hunt 1988). Similarly, HeH (helium hydride) produces five optical absorption bands, but not at the right wavelengths to explain the DQP bands (Ketterle, Figger, & Walther 1985).

C_2^- (Herzberg & Lagerqvist 1968; Lineberger & Patterson 1972) has a bandhead at 5416 Å, close to an observed DQP band centroid at 5400 Å. However, that C_2^- band is blue-shaded, not symmetric like the DQP band. Furthermore, the neighboring C_2^- bandheads are at 4902 Å and 5985 Å, respectively, which are not good fits to the neighboring DQP bands.

The rhombic C_4 isomer is predicted to produce an electronic band of comparable strength to the Swan bands (Muhlhauser et al. 2000; Kokkin, Bacskey, & Schmidt 2007) in the vicinity of 5450-5800 Å via absorption from the X^1A_g ground state to the $^1B_{1u}$ excited state (Masso et al. 2006). However, the band has not been observed experimentally and related vibronic band predictions have not been made. The linear isomer of C_4 produces UV/optical bands at 3340-3790 Å, but they are about 50 times weaker than the Swan bands (Linnartz et al. 2000; Muhlhauser et al. 2000). No information is available about optical bands of the branched C_4 isomer, which is thought to be a nearly planar tetrahedron (Hochlaf, Nicolas, & Poisson 2007). C_4 would be a long-shot explanation for the DQP bands, but the existing data do not rule it out. Absorption from all three C_4 isomers would be expected in that case. Bands from linear C_4 are not seen in one DQP WD with the required spectral coverage (Hintzen 1986), but the bands are expected to be weak.

Finally, for completeness we note that isotopically shifted Swan bands cannot explain the DQP bands: $^{13}\text{C}^{12}\text{C}$ and $^{13}\text{C}^{13}\text{C}$ have bands shifted about 8 Å and 16 Å *longward* in wavelength, respectively, from those of C_2 (King & Birge 1929; Swings 1943).

2.3. An Unknown Diatomic Molecule?

If we treat the DQP bands as being from an unknown diatomic molecule, we can infer some approximate characteristics of the two electronic states involved. We assume that the DQP centroid wavelengths given in Schmidt et al.

TABLE 2
BAND SYSTEM CONSTANTS

Band System	ΔE	ω_l	$\omega_l x_l$	ω_u	$\omega_u x_u$
DQp	19656	1395.3	-44.36	2201.9	173.4
Swan	19306.26	1641.33	11.65	1788.22	16.46
$C_2^- (X^2\Sigma_g^+, B^2\Sigma_u^+)$	18390.88	1781.04	11.58	1968.73	14.43

(1999) are the wavelengths of the (v_l, v_u) vibrational bands (0,2), (0,1), (0,0), (1,0) and (2,0) of the same electronic transition, where v_l and v_u are the initial and final vibrational quantum numbers. The wavenumber of the (v_l, v_u) vibronic transition can be approximated as

$$\omega_{lu} = \Delta E/hc + \omega_u(v_u + \frac{1}{2}) - \omega_u x_u(v_u + \frac{1}{2})^2 - \omega_l(v_l + \frac{1}{2}) + \omega_l x_l(v_l + \frac{1}{2})^2 \quad (1)$$

where $\Delta E = E_u - E_l$ is the (unknown) energy difference between the electronic states involved, h is Planck's constant, c is lightspeed and ω_u , $\omega_u x_u$, ω_l and $\omega_l x_l$ are constants to be determined (Herzberg 1950). A pure harmonic oscillator potential would have $\omega x=0$, while for realistic potentials there are likely to be additional higher-order terms; nonetheless, the approximation in Equation 1 is useful.

Five peculiar DQ bands have been observed, so we can use those five ω_{lu} values with their (assumed) associated v_l and v_u to solve for the five unknowns. Table 2, where they are compared with the corresponding parameters for the Swan bands and for the optical bands of C_2^- . Taking these coefficients at face value, the energy difference between the DQp electronic states is 1.8% larger than between the Swan band electronic states. The DQp ωx values are large relative to the ω values, indicating much more anharmonic potentials than for either state involved with the Swan bands. The smaller ω_l value for the DQp bands indicates a lower state with a potential energy curve broader than that of the Swan band lower state, and the larger ω_u value for the DQp bands indicates a upper state with a potential energy curve narrower than that of the Swan band upper state. Last but not least, the negative value of $\omega_l x_l$ is extremely unusual (Herzberg 1950). We can find only one diatomic molecule containing H, C or O with any transition characterized by a negative ωx ; namely, CsH (Huber & Herzberg 1979).

Thus, the characteristics of the DQp bands argue against attribution of the bands to an unidentified diatomic molecule. In deriving those characteristics, however, we did equate the band centroids with the wavelengths of transitions involving a $v = 0$ vibrational level. If that assumption is not correct, then the characteristics of the energy states involved may be less unusual. Since the long-wavelength edges of the DQp bands have wavelengths consistent with the $v = 0$ bandheads of the Swan system, it seems plausible that the DQp bands are the Swan bands, a possibility we now consider.

3. THE PECULIAR DQ BANDS: C_2 AS AN EXPLANATION

If the references cited in the sections 2.1 and 2.2 are correct (and for them to be wrong would require laboratory spectroscopy to have missed transitions as strong as the C_2 Swan bands), then the similarity of the bands in peculiar DQ WDs to those in normal DQ WDs suggests that C_2 produces the peculiar DQ bands. In this section we use observations and basic molecular physics to consider how C_2 might be producing the peculiar DQ bands. We begin by summarizing the salient features of the C_2 molecule and the Swan bands.

3.1. Basic Physics of C_2 and the Swan Bands

The electron configuration of the C_2 ground state ($X^1\Sigma_g^+$) can be approximated as $\sigma_{u2s}^2\pi_{u2p}^4$ (omitting the inner orbitals $\sigma_{g1s}^2\sigma_{u1s}^2\sigma_{g2s}^2$), while that of the Swan band lower ($a^3\Pi_u$) and upper ($d^3\Pi_g$) states are $\sigma_{u2s}^2\pi_{u2p}^3\sigma_{g2p}$ and $\sigma_{u2s}^*\pi_{u2p}^3\sigma_{g2p}^*$ respectively (Mulliken 1939). That is, the Swan bands are produced by vibronic transitions where an electron moves from a vibrational level in the σ_{2s}^* electronic orbital to one in the σ_{2p} orbital. (Unstarred orbitals are bonding orbitals, while starred orbitals are antibonding. The subscripts g and u indicate symmetry and antisymmetry, respectively, of the electron wavefunctions with respect to reflection through the center of the molecule.) Because of the transfer of an electron from an antibonding to a bonding orbital, Swan band absorption puts the C_2 molecule in an upper state where it has a 3.7% shorter equilibrium internuclear separation r_e than it did in the lower state (Mulliken 1939; Prasad & Bernath 1994).

The Swan bands are made up of many individual rovibronic transitions (transitions with simultaneous changes in rotational quantum number J , vibrational quantum number v , and electronic state). Each individual Swan band is characterized by a particular $\Delta v = v_l - v_u$ and consists of overlapping rovibronic bands with different (v_l, v_u) . Each rovibronic band consists of all possible rotational transitions for a particular vibronic transition (characterized by a given Δv and v_l). For example, the $\Delta v=0$ Swan band contains rovibronic bands (0,0), (1,1), etc.

Each rovibronic band consists of a P branch ($J \rightarrow J-1$) and an R branch ($J \rightarrow J+1$). For the Swan bands with $|\Delta v| \leq 2$, as $J = J_l$ increases with each rovibronic band the wavelengths of the corresponding R branch transitions continually decrease. In contrast, with increasing J the wavelengths of the corresponding P branch transitions first increase, then reach a maximum (forming the bandhead of the rovibronic band), and then continually decrease.

The Swan bands are usually said to be shaded to the blue, meaning that rovibronic bands with larger v_l have bandheads at shorter wavelengths. However, this is strictly true only for $v_l \leq 7 + 2\Delta v$: at sufficiently large v_l the rovibronic bandheads shift to longer wavelengths with increasing v_l .

The relative absorption strength of a particular Swan band rovibronic transition ($J_l \rightarrow J_u, v_l \rightarrow v_u$) depends on the population of the (J_l, v_l) level and the square of the overlap integral $\int \psi_l^* \psi_u d\vec{r}$, known as the Franck-Condon factor. Simply put, the more the maxima of the electron probability densities in the lower and upper rovibronic levels match up, the greater the probability of a transition between them.

3.2. Pressure-Shifted Swan Bands?

The high gravity of white dwarfs causes gravitational separation of elements. If there is substantial helium and hydrogen in a WD, the WD will have a hydrogen envelope atop a helium layer atop a carbon layer, etc. As white dwarfs cool below $T_{\text{eff}} \lesssim 16000$ K, the hydrogen and helium layers (or the helium layer alone, if hydrogen is absent) can become deeply convective if they are not too thick. Thus, some cool WDs have helium-dominated atmospheres with trace amounts of carbon ($10^{-7} - 10^{-2}$; Koester et al. 1982; Pelletier et al. 1986) as well as hydrogen ($10^{-6} - 10^{-1}$; Schmidt et al. 1995). Because He is predominantly neutral at such temperatures, the atmosphere of a cool He-rich WD is highly transparent in the optical and the photosphere is located relatively deep within the star, at high pressure ($P \simeq 10^{11}$ dyne $\text{cm}^{-2} = 10$ GPa; Jørgensen et al. 2000). The dominant source of opacity in such atmospheres is He^- (Jørgensen et al. 2000), with trace heavy elements such as carbon providing the donor electrons. A lower metal abundance should therefore decrease the atmospheric opacity, shifting the photosphere downwards, to higher pressure. As T_{eff} decreases in DQ WDs, the carbon abundance is observed to decrease due to a decreasing efficiency of convective carbon dredge-up (Dufour et al. 2005; Koester & Knist 2006). It is therefore at least plausible that the DQp bands could be Swan bands affected by high pressure.

The gas pressure in a WD is governed by the hydrostatic equation $dP_g/d\tau = g\rho/k$, where τ is the optical depth, g the acceleration due to gravity, ρ the density and k the total linear absorption coefficient from all sources of opacity (Allard & Wehrse 1990). If DQp bands are generated by C_2 at high pressure, then at $\tau \sim 1$ in a DQp WD atmosphere k must be larger, or g or ρ smaller, than at $\tau \sim 1$ in a DQ WD atmosphere. For a cool, He-rich WD to become a DQp WD, a low metal abundance might be needed, since that would reduce the availability of donor electrons and reduce the He^- opacity, thus shifting the photosphere to higher pressures. Alternatively, a larger value of g might be required, due to DQp WDs having typically higher masses than DQ WDs. However, there is no evidence that the latter is the case: Bergeron, Leggett, & Ruiz (2001) do not find systematically higher masses for DQp WDs as compared to DQ WDs, and there is some evidence that a subset of *normal* DQ WDs have systematically large masses (Dufour et al. 2005).

Pressure shifting of the Swan bands as an explanation for the DQp bands was originally suggested by Liebert & Dahn (1983) but seemingly ruled out by Bergeron et al. (1994). In the latter paper, the photospheric pressure in a model for the DQp WD LHS 1126 was found to be three times smaller than the photospheric pressures in the coolest normal DQ WDs analyzed by Wegner & Yackovich (1984). However, numerous inadequacies in current models of cool white dwarf atmospheres have recently come to light (e.g., Kowalski, Saumon, & Mazevet 2005; Dufour et al. 2007a). For LHS 1126 specifically, the large H/He ratio of $10^{-0.8}$ found by Bergeron et al. (1994) was shown by Wolff, Koester, & Liebert (2002) to grossly overpredict the Ly α absorption strength in that object, which is most consistent with H/He= $10^{-4.5}$. Furthermore, neither model correctly predicts the mid-infrared fluxes of LHS 1126 recently reported by Kilic et al. (2006). No current model can satisfactorily explain the entire spectral energy distribution of the DQp WD LHS 1126. Therefore, the conclusion that it has a lower photospheric pressure than some normal DQ WDs, and thus that the DQp bands cannot be pressure-shifted Swan bands, may have been premature.

As improved models of cool, He-rich WD atmospheres become available, it will be worth refitting well-observed DQ and DQp WDs to determine whether the DQp bands could be pressure-shifted Swan bands. For example, Homeier, Allard, & Allard (2007) have shown that at sufficiently high pressure, collisions of Na atoms with H_2 or He can shift Na I absorption shortwards as well as broaden it. It is worth investigating if collisions of C_2 with H_2 or He could produce a similar effect and, if so, at what pressures. (A 50 Å shortward shift of the Swan bands at a pressure of 10^{10} dynes cm^{-2} was reported by Bues (1999), but no details of the calculation were given.)

Theoretically, Lin (1973) has shown that pressure can shift vibronic bands either shortward or longward in wavelength, that the energy shift is identical for each band, and that such bands are likely to appear increasingly Gaussian at higher pressure. The DQp bands are in fact shifted by from the Swan bands by roughly identical energies ($+700 \pm 100$ cm^{-1}) and appear roughly Gaussian, so the DQp bands do possess some features of pressure-shifted bands.

Experimentally, H_2 and N_2 immersed in dense, high-pressure He show an increase in vibrational energy level spacing (Loubeyre, LeToullec, & Pinceaux 1992; Scheerboom, Michels, & Schouten 1996). The increase is due simply to compression of the molecule: shortening of the intramolecular bond leads to more energy being required to excite vibrations. Unfortunately, even assuming the same is true for C_2 , no rovibronic bands which could be used to measure such an increase appear within the DQp bands. Neither is experimental information available on vibronic band shifts for H_2 , N_2 or C_2 in He. However, in mixtures of 1% N_2 in low-temperature Ar, Kr or Xe, at least one N_2 vibronic band is seen to shift to *longer* wavelengths as a function of increasing pressure (Semling et al. 1997). The upper state involved in those N_2 transitions has a larger r_e than the lower state, so it is likely that the upper state undergoes greater compression (Lin 1973), making it more tightly bound and reducing the energy difference between it and the lower state. If that is the case, the Swan bands may behave oppositely (vibronic bands shifted shortwards), since the lower state involved is larger and thus likely to undergo greater compression under pressure.

Empirically, the DQp bands exhibit some characteristics consistent with being pressure-shifted Swan bands where the lower state involved is more affected by pressure than the upper state. As mentioned in the previous paragraph, the DQp bands show no evidence for bandheads. For the bandheads formed by the rotational P branches to disappear

without bandheads appearing in the R branches, the rotational constants in the (shifted) lower and upper Swan band states must be nearly equal: $B_l \simeq B_u$ (Herzberg 1950). Since $B \propto I^{-1}$, where $I \propto r_e^2$ is the moment of inertia perpendicular to the internuclear axis, nearly equal values of B require nearly equal internuclear separations in the two states. That requirement is consistent with the Swan band lower state being more affected by pressure than the upper state. Another expected consequence of more nearly equal internuclear separations is a shift in the peak absorption within each Swan band to shorter wavelengths due to smaller (larger) Franck-Condon factors for levels with small (large) v_l . This narrowing of the Condon parabola (Herzberg 1950; Cooper 1975) may also reduce the overall intensities of the $|\Delta v| \geq 2$ bands in DQp WDs relative to DQ WDs (see § 3.4).

In summary, it seems plausible that high pressures and temperatures could distort the Swan bands in such a manner as to produce the DQp bands. If detailed calculations or laboratory experiments show that pressure-shifted Swan bands do indeed resemble the DQp bands, the claim that DQp WDs do not have higher photospheric pressures than DQ WDs will need to be checked with better models of cool WD atmospheres.

3.3. Absorption from Vibrationally or Rotationally Excited C_2 ?

Generally speaking, absorption from rotationally or vibrationally excited levels of C_2 appears at shorter wavelengths than the Swan bandheads. Thus, as pointed out by Schmidt et al. (1995), such absorption might explain the DQp bands. We consider these possibilities in detail here.

Vibrational excitation of C_2 by itself will not suffice. For Swan bands with $\Delta v \leq 0$, absorption from $v_l \approx 7$ can match the DQp band centroids. However, for Swan bands with $\Delta v > 0$, the rovibronic bandheads never reach wavelengths as short as the DQp band centroids (Phillips & Davis 1968). Moreover, a very high temperature of $T_{vib} \gtrsim 17000$ K would be required to populate the $v_l=7$ level, as it is located ~ 12000 cm $^{-1}$ above the $v_l=0$ level. Furthermore, the $\Delta v = 0$ Swan band has very small Franck-Condon factors for $v_l > 3$, so vibrationally excited C_2 should produce a very weak $\Delta v = 0$ band. Lastly, in thermodynamic equilibrium, even if levels with $v_l \approx 7$ were populated, levels with $v_l < 0$ should be equally populated. That would yield absorption profiles *extended* to shorter wavelengths, but not *shifted* to shorter wavelengths.

Rotational excitation of C_2 could explain the DQp bands, since the $2J+1$ degeneracy of rotational levels yields level populations which peak at a nonzero J value. Since the DQp band profiles are quite smooth even at the location of Swan band rovibronic bandheads, the wavelength shift for the J_{peak} level in both the P and R branches must be larger than the wavelength separation of rovibronic bandheads. Such a shift requires $J_{peak} \gtrsim 45$ (Phillips & Davis 1968), corresponding to energies $\gtrsim 3600$ cm $^{-1}$ above the $J=0$ level, or $T_{rot} \gtrsim 5200$ K. Absorption from rotationally excited C_2 could be a plausible explanation for the DQp bands if C_2 absorption in a DQ WD occurs high in the atmosphere, so that T_{rot} is low, while the C_2 absorption in a DQp WD occurs deep in the atmosphere, so that T_{rot} is high. Such a scenario is broadly in agreement with the models of Bues (1999).

These features of Swan and DQp bands are illustrated in Figure 1, which shows partial spectra from the Sloan Digital Sky Survey (SDSS; York et al. 2000; Adelman-McCarthy et al. 2008) of two DQ WDs and the DQp WD SDSS J223224.00–074434.2 (Harris et al. 2003). The existence of the latter object proves that if the DQp bands are shifted Swan bands, the underlying physical mechanism does not shift the bands by only a single, fixed energy, as was believed to be the case at the time of the Schmidt et al. (1995) study. Furthermore, there is some indication in the spectrum of SDSS J223224.00–074434.2 that the rovibronic bandheads are not completely washed out. This suggests either a lower pressure or a lower T_{rot} in the line-forming region of SDSS J223224.00–074434.2 as compared to other DQp WDs where no sign of those bandheads remains. Note that $J_{peak} \gtrsim 20$ is required to shift Swan band absorption significantly away from the rovibronic bandheads, since those bandheads are formed by the P branch with $J \simeq 15$. (For $J_{peak} \lesssim 20$, the absorption will be extended to shorter wavelengths but the bandheads will not be shifted to shorter wavelengths.)

Detailed modeling of the bands in DQ and DQp WDs should be able to determine whether combined rotational and vibrational excitation at a single $T = T_{rot} = T_{vib}$ can explain the band shapes quantitatively as well as qualitatively. If so, it will be possible to determine the excitation temperature ranges seen in DQ and DQp WDs for comparison with models. If not, pressure-shifted Swan bands would seem to be the only viable explanation left for the DQp bands.

3.4. Magnetic Considerations

It is now feasible to predict the spectra of C_2 in the presence of magnetic fields of $\lesssim 10^7$ Gauss (Berdyugina, Berdyugin, & Pirola 2007), though no detailed calculations have been published for higher field strengths where the quadratic Zeeman effect becomes important. Such modeling is important because magnetic fields can shift the Swan bands to shorter wavelengths (Liebert et al. 1978), producing bands that resemble the (nonmagnetic) DQp bands. In a magnetic field, the P and R branches of the Swan bands become circularly polarized in opposite senses (Berdyugina et al. 2007). Because the P and R branches are not separated in wavelength, the net Swan band circular polarization signal is weak for fields $\lesssim 10^7$ Gauss (Schmidt et al. 2003). However, it can reach $\sim 10\%$ at $\gtrsim 10^8$ Gauss (Schmidt et al. 1999), which may be a result of quadratic Zeeman shifts.

Schmidt et al. (1999) suggested that DQp bands show weaker quadratic Zeeman shifts than the Swan bands do. However, this suggestion is not a certainty, given the possibility of a range of magnetic field strengths (as well as geometries and orientations) combined with a range of DQp band centroid shifts due to pressure, rotational excitation, or both. For example, it may be that a peculiar DQ WD with an intrinsically moderate band centroid shift *and* a moderate magnetic field can have a spectrum similar to a normal DQ WD with a strong magnetic field. Specifically,

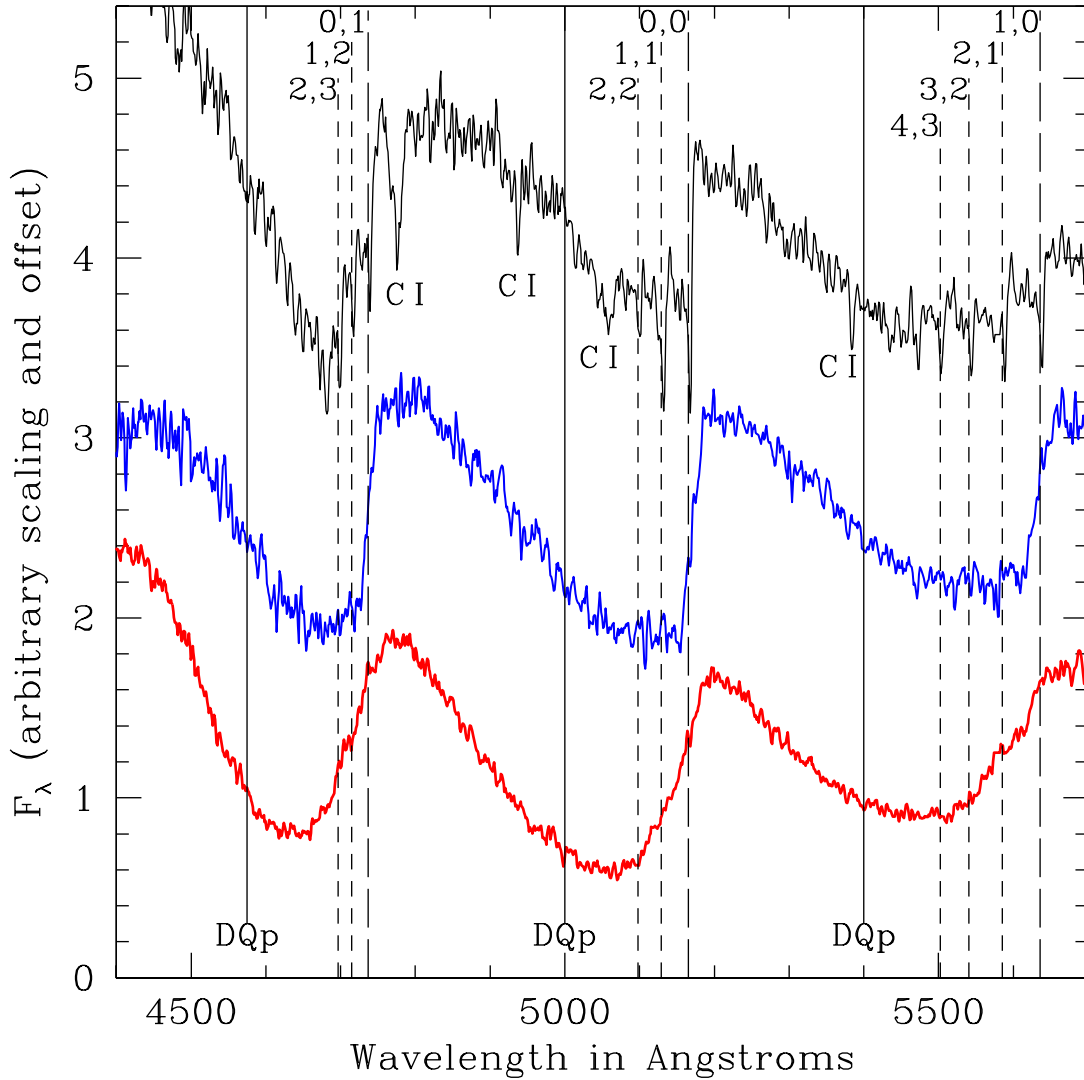


FIG. 1.— Partial spectra of DQ and DQp WDs from the SDSS. Solid vertical lines show the DQp band centroid wavelengths from Schmidt et al. (1995). Dashed lines show bandhead wavelengths of the Swan band system, while dotted lines show rovibronic bandhead wavelengths within different Swan bands; all lines are labeled with (v_l, v_u) . At the top is the DQ WD SDSS J104559.13+590448.3 (thin line), which shows narrow absorption in the Swan bands as well as from C I. In the middle is the DQ WD SDSS J102801.74+351257.9 (thick blue line), which has excited levels of C₂ sufficiently populated that different rovibronic bands are blended together, as well as some line broadening (pressure broadening?) which extends the absorption profiles slightly longward of the Swan bandheads. At the bottom is the DQp WD SDSS J223224.00−074434.2 (thicker red line), whose absorption profiles show a similar amount of line broadening along with a band centroid shift about half that seen in the DQp stars of Schmidt et al. (1995). Its absorption profiles are smooth but not featureless; the slope of a profile tends to change near the wavelength of a Swan band rovibronic bandhead (dotted lines), suggesting that the DQp bands are modified Swan bands.

Schmidt et al. (1999) suggest that LP 790−29 is a magnetic DQ and LHS 2229 a magnetic DQp. We suggest that *both* might be DQp WDs, with LHS 2229 having the stronger magnetic field of the pair but LP 790−29 having a much larger intrinsic DQp band centroid shift. The relative field strength estimate is based on the maximum change in circular polarization between wavelengths outside and inside the Swan bands being larger in LHS 2229 than in LP 790−29 (25% vs. 10%); of course, the change in circular polarization could be affected by magnetic field geometry and orientation as well. The intrinsic DQp band centroid shift estimate assumes that the pronounced weakness of the $|\Delta v| \geq 2$ bands in LP 790−29 is due to smaller Franck-Condon factors between energy states with reduced internuclear separations (§ 3.2). Similar conclusions might apply to the similar WDs from Schmidt et al. (2003): the band centroid shifts in SDSS J133359.86+001654.8 are larger than in LHS 2229, and those in SDSS J111341.33+014641.7 are larger than in LP 790−29, but each SDSS object is *less* polarized than its non-SDSS counterpart. We suggest that those two SDSS objects have considerably larger intrinsic DQp band centroid shifts but somewhat smaller magnetic shifts than their respective non-SDSS counterparts, leading to greater overall absorption band shifts.

Progress on understanding magnetic DQ WDs may therefore require calculations which simultaneously incorporate the effects of pressure, rotational (and vibrational) excitation and magnetic field strengths above 10^7 Gauss.

4. CONCLUSIONS

We have shown that the molecular absorption bands in peculiar DQ WDs are very unlikely to be produced in any molecule other than C_2 (§ 2). We have considered how the DQp bands can be explained as modified Swan bands (§ 3) and conclude that they could either be pressure-shifted Swan bands (as originally suggested by Liebert & Dahn 1983) or Swan band absorption from highly rotationally excited levels, or both. Regardless, a continuum of increasingly shifted and reshaped bands is expected to be observed in DQp WDs, in agreement with recent observations (§ 3.3).

One implication of our result is that the putative absence of WDs with $T_{\text{eff}} \lesssim 6000$ K which exhibit molecular carbon absorption (Dufour et al. 2005) is not real — the DQp WDs are such objects. Another implication is that understanding the spectra of magnetic DQ WDs may require models which simultaneously account for the effects of pressure, rotational excitation and magnetic fields on C_2 absorption.

Theoretical and experimental investigations of the properties of C_2 in high-pressure, high-temperature helium are needed to determine if pressure-shifted Swan bands resemble the DQp bands. If they do not, then the only remaining explanation for the DQp bands seems to be that they arise in rotationally excited C_2 ($J_{\text{peak}} \gtrsim 45$). That scenario would require a higher T_{rot} in DQp WDs than in DQ WDs, perhaps due to C_2 absorption arising deeper in the photosphere in DQp WDs (Bues 1999).

Even if pressure-shifted Swan bands are found to resemble the DQp bands, existing models of WD atmospheres suggest that DQp WDs do not have higher photospheric pressures than DQ WDs and thus that the peculiar DQ bands are not pressure-shifted Swan bands. Nonetheless, since there are known shortcomings in existing models of cool, He-rich WD stellar atmospheres, that tentative conclusion needs to be revisited when improved models become available.² If DQp WDs do have higher photospheric pressures than DQ WDs, the reason may be that low metal abundances reduce the He^- opacity by restricting the availability of donor electrons.

Whichever explanation of the DQp bands is eventually confirmed, with accurate theoretical models it should be possible to use C_2 absorption band profiles as a sort of barometer to constrain both the pressure and the rotational temperature of C_2 in the line-forming regions of DQ and DQp WD atmospheres. For example, examination of Swan band fits to DQ WD absorption profiles shows that the observed profiles are often more rounded than predicted (Dufour et al. 2005; Koester & Knist 2006). Thus, the observed profiles may provide evidence for an increasing J_{peak} or an increasing pressure shift with decreasing T_{eff} even among normal DQ WDs. However, these discrepancies could simply be due to imprecise knowledge of Swan band absorption parameters or to inexact treatment of the WD atmospheres or of C_2 itself. For example, Dufour et al. (2005) calculate C_2 line profiles using the impact approximation, which is known to break down in dense DQ WD atmospheres where the mean distance between particles is comparable to the particle size (Koester, Weidemann, & Zeidler 1982).

Observationally, more and better parallax values for DQ and DQp WDs would provide information on the range of masses seen in each type of WD and help determine what contribution different values of g make to the DQp phenomenon. It might also be useful to search for and study other C_2 bands in normal and peculiar DQ WDs. Whatever physical effect transforms the Swan bands into the DQp bands, its effect on other C_2 energy states, and thus other C_2 bands, may be different and may serve as a clue to its origin.

We dedicate this paper to Dr. Ralph Nicholls, who passed away in January 2008 after working at York University on C_2 and many other molecules since before either of this paper's authors were born. We thank H. Harris and G. Schmidt for discussions and M. Horbatsch for refusing to believe that the spectrum of C_2H was unknown. PBH acknowledges support from York University and NSERC. This research would not have been feasible without the collections of the York University Libraries and the Ontario Council of University Libraries.

² More speculatively, it would also be worth investigating the properties of carbon-atmosphere WDs (Dufour et al. 2007b) at low T_{eff} , to see if they have high photospheric pressures. Although Dufour et al. (2007b) state that no carbon-atmosphere WD is known at $T_{\text{eff}} < 15,000$ K, carbon-atmosphere WDs were not thought to exist at all before their recent discovery. We cannot be confident that all carbon-atmosphere WDs develop a helium atmosphere as they cool until the origin of such objects is better understood. If predictions can be made of the spectra of carbon-atmosphere WDs at low T_{eff} , the SDSS provides a large database in which to search for objects with such spectra.

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